STN SEARCH TRANSCRIPT 10/681,205

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 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  JAN 17  Pre-1988 INPI data added to MARPAT
 NEWS  4  FEB 21  STN AnaVist, Version 1.1, lets you share your STN AnaVist
                  visualization results
 NEWS  5  FEB 22  The IPC thesaurus added to additional patent databases on STN
 NEWS  6  FEB 22  Updates in EPFULL; IPC 8 enhancements added
 NEWS  7  FEB 27  New STN AnaVist pricing effective March 1, 2006
 NEWS  8  MAR 03  Updates in PATDPA; addition of IPC 8 data without attributes
 NEWS  9  MAR 22  EMBASE is now updated on a daily basis
 NEWS 10  APR 03  New IPC 8 fields and IPC thesaurus added to PATDPAFULL
 NEWS 11  APR 03  Bibliographic data updates resume; new IPC 8 fields and IPC
                  thesaurus added in PCTFULL
 NEWS 12  APR 04  STN AnaVist $500 visualization usage credit offered
 NEWS 13  APR 12  LINSPEC, learning database for INSPEC, reloaded and enhanced
 NEWS 14  APR 12  Improved structure highlighting in FQHIT and QHIT display
                  in MARPAT
 NEWS 15  APR 12  Derwent World Patents Index to be reloaded and enhanced during
                  second quarter; strategies may be affected
 NEWS 16  MAY 10  CA/CAplus enhanced with 1900-1906 U.S. patent records
 NEWS 17  MAY 11  KOREAPAT updates resume
 NEWS 18  MAY 19  Derwent World Patents Index to be reloaded and enhanced

 NEWS EXPRESS  FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
               V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
               http://download.cas.org/express/v8.0-Discover/

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that
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  COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

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  to STN.

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  Thank you in advance for your participation.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:39:19 ON 26 MAY 2006

=> FILE REG
COST IN U.S. DOLLARS                                 SINCE FILE     TOTAL
                                                          ENTRY   SESSION
FULL ESTIMATED COST                                        0.21      0.21

FILE 'REGISTRY' ENTERED AT 12:39:23 ON 26 MAY 2006
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES:    25 MAY 2006  HIGHEST RN 885654-58-0
DICTIONARY FILE UPDATES:   25 MAY 2006  HIGHEST RN 885654-58-0

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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*******************************************************************
*                                                                 *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,  *
* effective March 20, 2005.  A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*                                                                 *
*******************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

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=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=>
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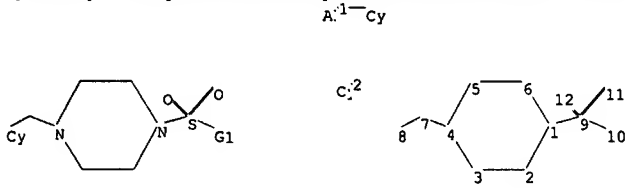
Uploading C:\Program Files\Stnexp\Queries\HABTE SULFONYL RCE.str



chain nodes :
7 8 9 10 11 12 13 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
1-9 4-7 7-8 9-10 9-11 9-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-9 2-3 3-4 4-5 4-7 5-6 7-8 9-10 9-11 9-12 13-14
isolated ring systems :
containing 1 :

G1:[*1],[*2]

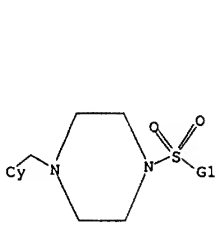
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom
Generic attributes :
8:
Type of Ring System : Polycyclic
13:
Saturation : Unsaturated
14:
Saturation : Unsaturated
Type of Ring System : Polycyclic
15:
Type of Ring System : Polycyclic

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> D L1
L1 HAS NO ANSWERS
L1 STR



G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 12:39:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2567 TO ITERATE

77.9% PROCESSED 2000 ITERATIONS 42 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 48301 TO 54379
PROJECTED ANSWERS: 638 TO 1518

L3 42 SEA SSS SAM L1

=> FILE CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	0.65

FILE 'CAPLUS' ENTERED AT 12:39:45 ON 26 MAY 2006
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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006 (20060525/ED)

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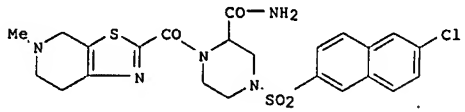
=> S L3
L4 10 L3

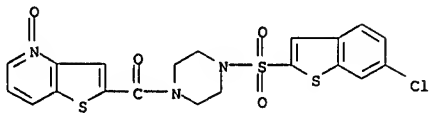
=> D 1-10 IBIB ABS HITSTR

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:64500 CAPLUS
DOCUMENT NUMBER: 144:205149
TITLE: Design, synthesis, and biological activity of novel factor Xa inhibitors: Improving metabolic stability by S1 and S4 ligand modification
AUTHOR(S): Komoriya, Satoshi; Kobayashi, Shozo; Osanai, Ken; Yoshino, Toshiharu; Nagata, Tsutomu; Haginoya, Noriyasu; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagahara, Takayasu; Suzuki, Makoto; Shimada, Takashi; Watanabe, Kengo; Isobe, Yumiko; Furugoori, Taketoshi
CORPORATE SOURCE: Tokyo R&D Center, Daiichi Pharmaceutical Co. Ltd, 16-13, Kita-Kasai 1-Chome, Edogawa-ku, Tokyo, 134-8630, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(5), 1309-1330
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

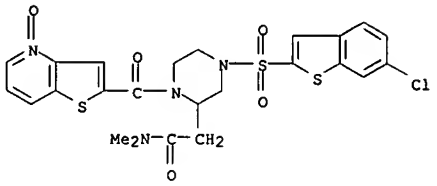


I

AB Serine protease factor Xa (fXa) inhibitor I showed good ex vivo anti-fXa activity upon oral administration in rats. However, it has been revealed that I had low metabolic stability against human liver microsomes. To improve the metabolic stability, we attempted to modify the S1 and S4 ligands of I. These modifications resulted in a compound which exhibited selective anti-fXa activity and excellent anti-coagulation activity.
IT **875573-53-8P 875573-54-9P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(factor Xa inhibitors with improved metabolic stability)
RN 875573-53-8 CAPLUS
CN Piperazine, 1-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-4-[(4-oxidothieno[3,2-b]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

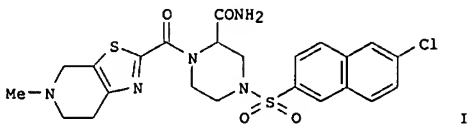


RN 875573-54-9 CAPLUS
CN 2-Piperazineacetamide, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-1-[(4-oxidothieno[3,2-b]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:747454 CAPLUS
DOCUMENT NUMBER: 141:395464
TITLE: Synthesis and Conformational Analysis of a Non-Amidine Factor Xa Inhibitor That Incorporates 5-Methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine as S4 Binding Element
AUTHOR(S): Haginoya, Noriyasu; Kobayashi, Syozo; Komoriya, Satoshi; Yoshino, Toshiharu; Suzuki, Makoto; Shimada, Takashi; Watanabe, Kengo; Hirokawa, Yumiko; Furugori, Taketoshi; Nagahara, Takayasu
CORPORATE SOURCE: Medicinal Chemistry Research Laboratory, Daiichi Pharmaceutical Co. Ltd, Edogawa-ku, Tokyo, 134-8630, Japan
SOURCE: Journal of Medicinal Chemistry (2004), 47(21), 5167-5182
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:395464
GI



I

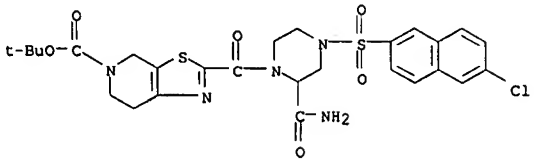
AB Our exploratory study was based on the concept that a non-amidine factor Xa (fXa) inhibitor is suitable for an orally available anticoagulant. We synthesized and evaluated a series of N-(6-chloronaphthalen-2-yl)sulfonylpiperazine derivs. incorporating various fused-bicyclic rings containing an aliphatic amine expected to be S4 binding element. Among this series, 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine type I displayed orally potent anti-fXa activity and evident prolongation of prothrombin time (PT) with the moderate bioavailability in rats. The X-ray crystal anal. afforded an obvious binding mode that

5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine and 6-chloronaphthalene resp. bound to S4 and S1 subsites. In this X-ray study, we discovered a novel intramol. S-O close contact. Ab initio energy calcns. of model compds. deduced that conformers with the most close S-O proximity were most stable. The Mulliken population anal. proposed that this energy profile was caused by both of electrostatic S-O affinity and N-O repulsion. The results of these calcns. and X-ray anal. suggested a possibility that the restricted conformation effected the affinity to S4 subsite of fXa.

IT **222987-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, factor Xa inhibition activity and structure-activity relationship of (chloronaphthalenylsulfonyl)piperazines bearing fused-heterobicyclic rings)

RN 222987-45-3 CAPLUS

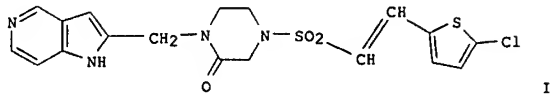
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:89919 CAPLUS
DOCUMENT NUMBER: 138:247939
TITLE: Discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand
AUTHOR(S): Choi-Sledeski, Yong Mi; Kearney, Robert; Poli, Gregory; Pauls, Henry; Gardner, Charles; Gong, Yong; Becker, Michael; Davis, Roderick; Spada, Alfred; Liang, Guyan; Chu, Valeria; Brown, Karen; Collussi, Dennis; Leadley, Robert, Jr.; Rebello, Sam; Moxey, Phillip; Morgan, Suzanne; Bentley, Ross; Kasiewski, Charles; Maignan, Sebastien; Guilloteau, Jean-Pierre; Mikol, Vincent
CORPORATE SOURCE: Department of Medicinal Chemistry, Aventis Pharmaceuticals, Bridgewater, NJ, 08807-0800, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(5), 681-684
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:247939
GI



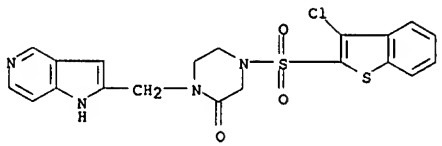
I

AB The discovery and SAR of ketopiperazino methylazaindole factor Xa inhibitors are described. Structure-activity data suggesting that this class of inhibitors does not bind in the canonical mode were confirmed by an X-ray crystal structure showing the neutral haloarom. bound in the S1 subsite. The most potent azaindole (I, RPR209685) is selective against related serine proteases and attains higher levels of exposure upon oral dosing than comparable benzamidines and benzamidine isosteres. Compound I was efficacious in the canine AV model of thrombosis.

IT **234100-32-4P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand)

RN 234100-32-4 CAPLUS

CN Piperazinone, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:769282 CAPLUS
DOCUMENT NUMBER: 135:313616
TITLE: Heterocyclic sulfonyl compounds and activated blood coagulation factor X (FXa) inhibitors containing them
INVENTOR(S): Kobayashi, Shozo; Komoritani, Satoshi; Haginoya, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Yoshikawa, Kenji; Muto, Akira; Ozanai, Takeshi; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagata, Tsutomu
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 304 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001294572	A2	20011023	JP 2000-38100	20000209

PRIORITY APPLN. INFO.: JP 2000-38100 20000209
OTHER SOURCE(S): MARPAT 135:313616

AB Pharmaceuticals, useful for prevention and/or treatment of thrombus and embolus, contain Q1Q2T1SO2QA [I; Q1 = (un)substituted bicyclic or

tricyclic group; Q2 = single bond, O, S, C1-6 alkylene, etc.; Q3 = N-containing cyclic group; QA = (un)substituted (hetero)arylalkenyl, bicyclic or tricyclic group, etc.; T1 = CO, (un)substituted methylene, etc.], their salts, or solvates. (2RS)-2-(N-tert-butoxycarbonylaminomethyl)-6-methoxycarbonyl-1,2,3,4-tetrahydronaphthalene was treated with NaOH, condensed with 1-[(6-chloronaphthalen-2-yl)sulfonyl]piperazine.HCl, and deprotected to give (RS)-I.HCl (Q1 = 6-aminomethyl-5,6,7,8-tetrahydronaphthalen-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl). I.HCl (Q1 = 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl) in vitro inhibited human FXa with IC50 of 20 nM.

IT **259805-94-2P 259806-37-6P 259806-48-9P**
259806-67-2P 259806-89-8P 259806-92-3P
259807-04-0P 368439-26-3P 368439-42-3P
368439-49-0P 368439-57-0P 368439-65-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic sulfonyl compds. as activated blood coagulation factor X inhibitors)

RN 259805-94-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[(4,5,6,7-tetrahydro-4-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 259805-93-1
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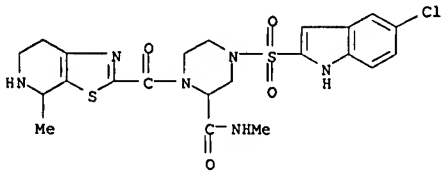
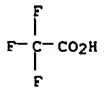
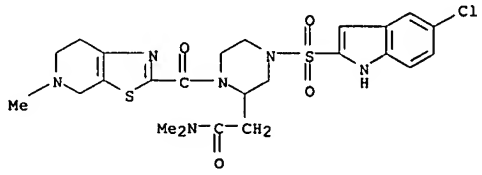


CM 2

CRN 76-05-1
CMF C2 H F3 O2

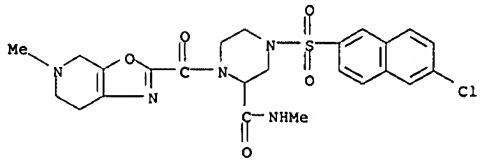


RN 259806-37-6 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N,N-dimethyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

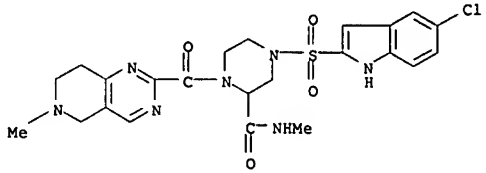


● HCl

RN 259806-48-9 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-N-methyl-1-[(4,5,6,7-tetrahydro-5-methyloxazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

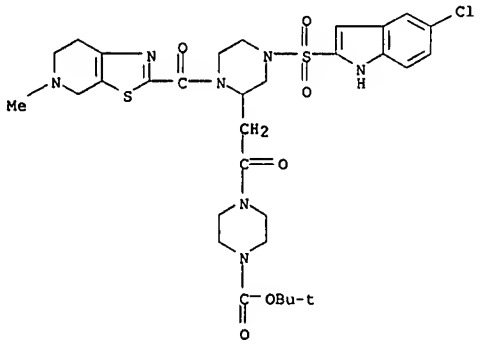


RN 259806-67-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[(5,6,7,8-tetrahydro-6-methylpyrido[4,3-d]pyrimidin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

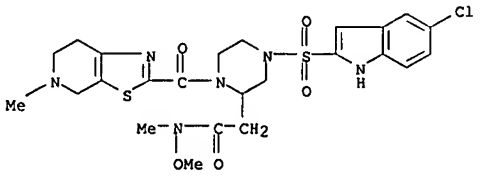


● HCl

RN 259806-89-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-2-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

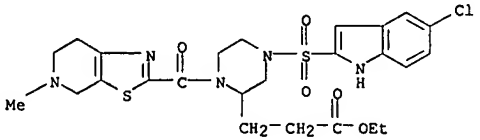


RN 259806-92-3 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methoxy-N-methyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

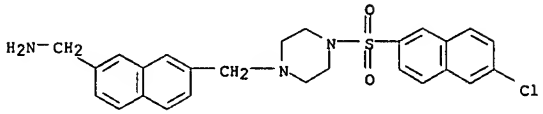


● HCl

RN 259807-04-0 CAPLUS
CN 2-Piperazinepropanoic acid, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

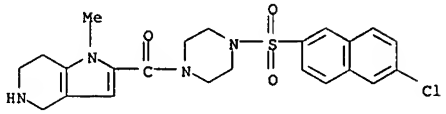


RN 368439-26-3 CAPLUS
CN Piperazine, 1-[[7-(aminomethyl)-2-naphthalenyl]methyl]-4-[(6-chloro-2-naphthalenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



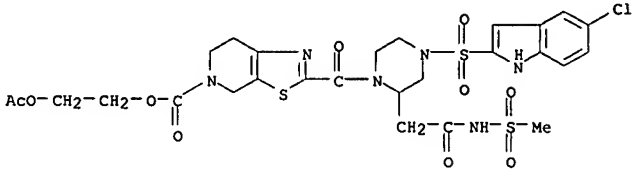
● HCl

RN 368439-42-3 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-1-methyl-1H-pyrrolo[3,2-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

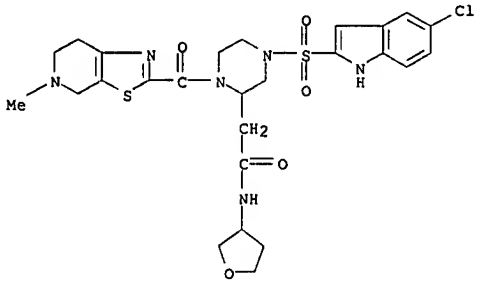


● HCl

RN 368439-49-0 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[4-[(5-chloro-1H-indol-2-yl)sulfonyl]-2-[2-[(methylsulfonyl)amino]-2-oxoethyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 2-(acetyloxy)ethyl ester (9CI) (CA INDEX NAME)

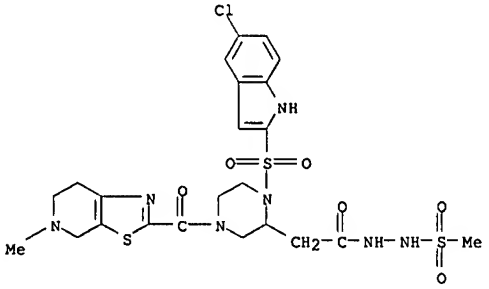


RN 368439-57-0 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-(tetrahydro-3-furanyl)-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



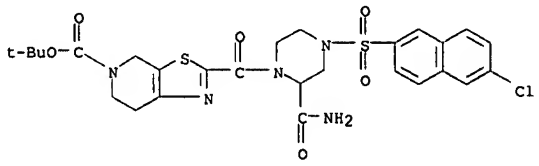
● HCl

RN 368439-65-0 CAPLUS
CN 2-Piperazineacetic acid, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, 2-(methylsulfonyl)hydrazide, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

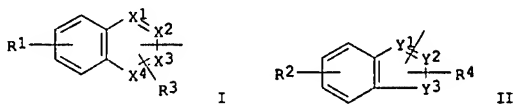
IT **222987-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic sulfonyl compds. as activated blood coagulation factor X inhibitors)
RN 222987-45-3 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



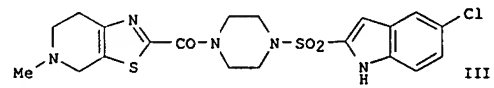
L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:636077 CAPLUS
DOCUMENT NUMBER: 135:211057
TITLE: Preparation of N-(tetrahydrothiazolo[5,4-c]pyridin-2-ylcarbonyl)piperazine derivatives and N-(4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-ylmethyl)pyrrolidine derivative and method for inhibiting trypsin-type serine proteases
INVENTOR(S): Komoriya, Satoshi; Haginoya, Noriyasu; Suzuki, Makoto
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 234 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062763	A1	20010830	WO 2001-JP1344	20010223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 2000-54370 A 20000225
GI



I II



III

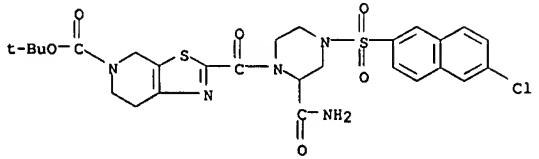
AB Trypsin-type serine protease inhibitors are compds. having groups

represented by the general formula (I) or (II) (wherein R1 and R2 are each hydrogen, C1-3 alkyl, halo, C2-3 alkenyl, or ethynyl; or R3 and R4 are each hydrogen, hydroxyl, or amino; X1, X2, X3 and X4 are each CH or N; Y1 and Y2 are each CH or N; and Y3 is NH, O or S). When such a compound is made to act on a trypsin-type serine protease, e.g. factor Xa (Fxa), the group enters the S1 pocket to thereby exert an inhibitory activity against the protease. Thus, to a solution of 400 mg 1-[(5-chloroindol-2-yl)sulfonyl]piperazine in 100 mL DMF were added 1-hydroxybenzotriazole 10.5, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride 194, lithium 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridinecarboxylate 175, and N-methylmorpholine 86.8 mg, and the resulting mixture was stirred at room temperature for 10 h to give 1-[(5-chloroindol-2-yl)sulfonyl]-4-(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-ylcarbonyl)piperazine hydrochloride (III.HCl). III.HCl showed IC50 of 0.005 μM against human FXa. X-ray crystallog. anal. of the complexes of human Gla domain-deficient β-FXa with the above compds. showed that bicyclic aromatic group (e.g. naphthalenyl) and aromatic heterocyclyl group (e.g. chloroindolyl) entered into the S1 pocket of the Fxa.

IT **222987-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (tetrahydrothiazolo[c]pyridinylcarbonyl)piperazine derivs. and (tetrahydrothieno[c]pyridinylmethyl)pyrrolidine derivative and method for inhibiting trypsin-type serine proteases)

RN 222987-45-3 CAPLUS

CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:78383 CAPLUS

DOCUMENT NUMBER: 134:163059

TITLE: Substituted piperazinone derivatives and other oxoazaheterocyclyl compounds useful as factor Xa/IIa inhibitors

INVENTOR(S): Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls, Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aiwen; Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.

PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA

SOURCE: PCT Int. Appl., 460 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

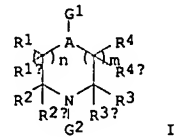
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007436	A2	20010201	WO 2000-IB1156	20000726
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2382755	AA	20010201	CA 2000-2382755	20000726
BR 2000013179	A	20020402	BR 2000-13179	20000726
EP 1208097	A2	20020529	EP 2000-951781	20000726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200225	T2	20020621	TR 2002-200200225	20000726
JP 2003508353	T2	20030304	JP 2001-512520	20000726
EE 200200045	A	20030616	EE 2002-45	20000726
AU 773227	B2	20040520	AU 2000-64628	20000726
NO 2002000214	A	20020402	NO 2002-214	20020115
BG 106340	A	20021031	BG 2002-106340	20020122
ZA 2002000543	A	20030623	ZA 2002-543	20020122

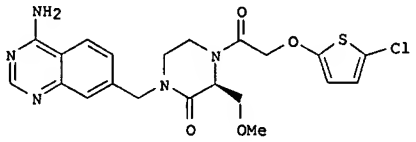
PRIORITY APPLN. INFO.: US 1999-363196 A 19990728
WO 2000-IB1156 W 20000726

OTHER SOURCE(S): MARPAT 134:163059

GI



I

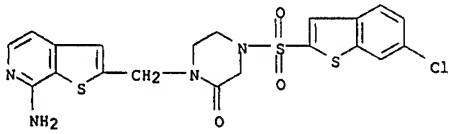


II

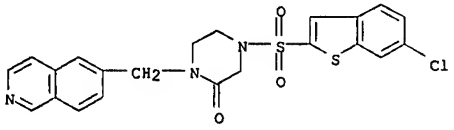
AB The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH or N; G1 and G2 = L1Cy1 or L2Cy2; Cy1 and Cy2 = (un)substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.; L1 = null, O, S, SO, SO2, or (un)substituted sulfamoyl, methylene, (alkyl)keto(alkyl), carbamoyl, etc.; L2 = null or linking group; R1, R1a, R2, R2a, R3, R3a, R4, R4a = independently H, carboxy, alkoxycarbonyl, alkyl, (hetero)aryl, aralkyl, heteroarylalkyl, etc.; m and n = independently 0-2]. The compds. inhibit factor Xa (no data) and factor IIa, and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 1600 invention compds. and several hundred intermediates. For instance, condensation of 5-chloro-2-thienyloxyacetic acid with the corresponding N-benzyloxycarbonyl-protected piperazinone derivative (prepns. given), using DIPEA and TBTU in DMF, gave II.

IT **234099-55-9P 234099-62-8P 234100-32-4P**
234100-58-4P 234105-43-2P 323587-45-7P
323593-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa/IIa inhibitors)

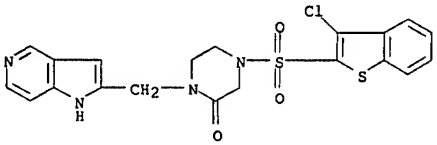
RN 234099-55-9 CAPLUS
CN Piperazinone, 1-[(7-aminothieno[2,3-c]pyridin-2-yl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]- (9CI) (CA INDEX NAME)



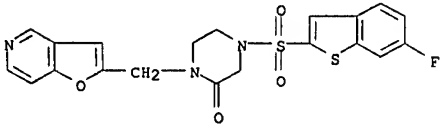
RN 234099-62-8 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(6-isoquinolinylmethyl)- (9CI) (CA INDEX NAME)



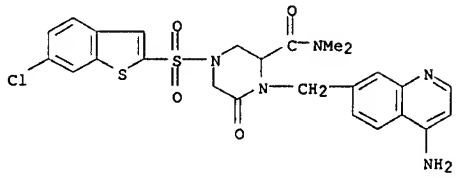
RN 234100-32-4 CAPLUS
CN Piperazinone, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



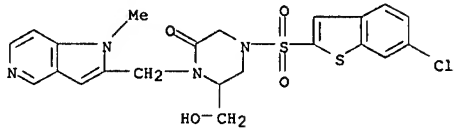
RN 234100-58-4 CAPLUS
CN Piperazinone, 4-[(6-fluorobenzo[b]thien-2-yl)sulfonyl]-1-(furo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234105-43-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-[(4-amino-7-quinolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-6-oxo- (9CI) (CA INDEX NAME)

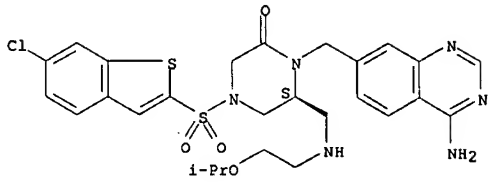


RN 323587-45-7 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-6-(hydroxymethyl)-1-[(1-methyl-1H-pyrrolo[3,2-c]pyridin-2-yl)methyl]- (9CI) (CA INDEX NAME)



RN 323593-63-1 CAPLUS
CN Piperazinone, 1-[(4-amino-7-quinazolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-6-[[[2-(1-methylethoxy)ethyl]amino]methyl]-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



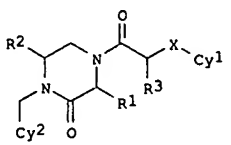
L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2000:384179 CAPLUS
DOCUMENT NUMBER:	133:30741
TITLE:	Substituted piperazinone derivatives and other oxoazaheterocyclyl compounds useful as factor Xa inhibitors
INVENTOR(S):	Ewing, William R.; Becker, Michael R.; Myers, Michael R.; Spada, Alfred P.
PATENT ASSIGNEE(S):	Aventis Pharmaceuticals Products Inc., USA
SOURCE:	PCT Int. Appl., 219 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English

FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000032590	A1	20000608	WO 1999-US28074	19991124
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
WO 9937304	A1	19990729	WO 1999-US1682	19990127
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2003529531	T2	20031007	JP 2000-585232	19991124
PRIORITY APPLN. INFO.:			US 1998-110012P	A2 19981125
			WO 1999-US1682	A2 19990127
			US 1999-313611	A2 19990518
			US 1999-363196	A2 19990728
			US 1998-72707P	A2 19980127
			WO 1999-US28074	W 19991124

OTHER SOURCE(S): MARPAT 133:30741
GI



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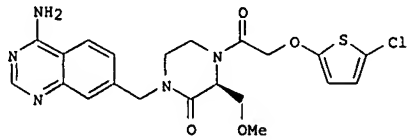
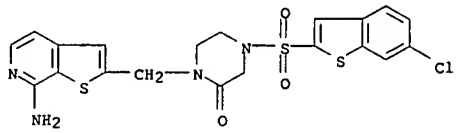


II

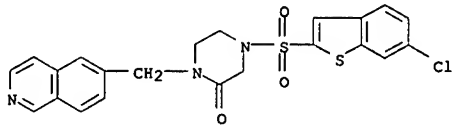
AB The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein R1 = H, alkyl, aryl, aralkyl, heteroaryl, heteroarylalkyl, alkoxy, aminoalkyl, CH2OZ, CH(CH3)OZ; R2 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroarylalkyl; R3 = H or Me; X = N or O; Z = lower alkyl or alkoxycarbonylalkyl; Cyl = (un)substituted aryl, (un)substituted heteroaryl; Cy2 = (un)substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.]. The compds. inhibit factor Xa (no data), and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 780 invention compds., approx. 50 of which are also claimed, and several hundred intermediates. For instance, condensation of 5-chloro-2-thienyloxyacetic acid with the corresponding N-benzyloxycarbonyl-protected piperazinone derivative (prepns. given), using DIPEA and TBTU in DMF, gave the preferred title compound II.

IT **234099-55-9P 234099-62-8P 234100-32-4P 234100-58-4P 234105-43-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa inhibitors)

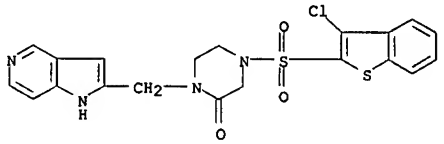
RN 234099-55-9 CAPLUS
CN Piperazinone, 1-[(7-aminothieno[2,3-c]pyridin-2-yl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]- (9CI) (CA INDEX NAME)



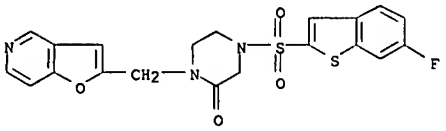
RN 234099-62-8 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(6-isoquinolinylmethyl)- (9CI) (CA INDEX NAME)



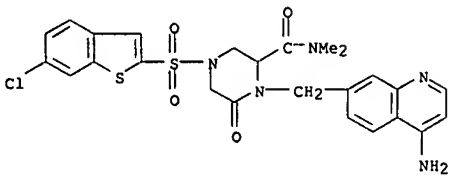
RN 234100-32-4 CAPLUS
CN Piperazinone, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234100-58-4 CAPLUS
CN Piperazinone, 4-[(6-fluorobenzo[b]thien-2-yl)sulfonyl]-1-(furo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234105-43-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-[(4-amino-7-quinolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:133658 CAPLUS
DOCUMENT NUMBER: 132:194391
TITLE: Preparation of sulfonyl moiety-containing heterocyclic compounds as factor Xa inhibitors
INVENTOR(S): Kobayashi, Syozo; Komoriya, Satoshi; Haginoya, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Nagata, Tsutomu; Horino, Haruhiko; Ito, Masayuki; Mochizuki, Akiyoshi
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 883 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

APPLICANTS

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009480	A1	20000224	WO 1999-JP4344	19990811
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2000119253	A2	20000425	JP 1999-226878	19990810
CA 2340100	AA	20000224	CA 1999-2340100	19990811
AU 9951963	A1	20000306	AU 1999-51963	19990811
EP 1104754	A1	20010606	EP 1999-937024	19990811
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2000143623	A2	20000526	JP 1999-242814	19990830
US 6747023	B1	20040608	US 2001-762888	20010212
US 2004082611	A1	20040429	US 2003-681205	20031009

PRIORITY APPLN. INFO.:
JP 1998-237449 A 19980811
JP 1998-244175 A 19980828
JP 1998-251674 A 19980904
WO 1999-JP4344 W 19990811
US 2001-762888 A3 20010212

OTHER SOURCE(S): MARPAT 132:194391

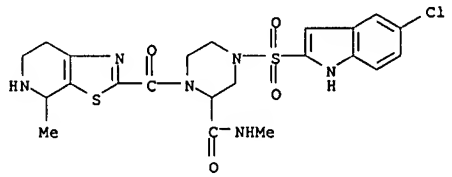
AB The title compds. Q1Q2T1Q3SO2QA [wherein Q1 is an optionally substituted, saturated or unsatd., five- or six-membered cyclic hydrocarbon group, a five- or six-membered heterocyclic group, or the like; Q2 is a single bond, oxygen, sulfur, C1-C6 alkylene or the like; Q3 is a heterocyclic ring (represented by several generic structures); QA is optionally substituted arylalkenyl, heteroarylalkenyl or the like; and T1 is carbonyl or the like] are prepared These compds. have potent factor Xa inhibiting effects and promptly exert satisfactory and persistent antithrombotic effects through oral administration, thus being useful as anticoagulant agents little accompanied with side effects. Several compds. of this invention in vitro showed IC50 values of 0.7 nM to 4.7 nM against factor Xa.

IT **259805-94-2P 259805-95-3P 259806-37-6P 259806-48-9P 259806-67-2P 259806-89-8P 259806-92-3P 259807-04-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonyl moiety-containing heterocyclic compds. as factor Xa inhibitors)

RN 259805-94-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[(4,5,6,7-tetrahydro-4-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

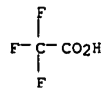
CM 1

CRN 259805-93-1
CMF C22 H25 Cl N6 O4 S2

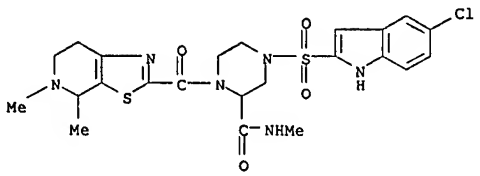


CM 2

CRN 76-05-1
CMF C2 H F3 O2

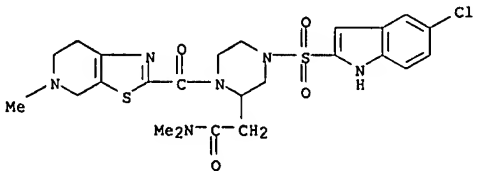


RN 259805-95-3 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[(4,5,6,7-tetrahydro-4,5-dimethylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



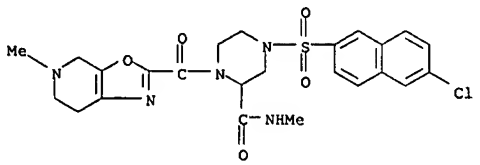
● HCl

RN 259806-37-6 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N,N-dimethyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

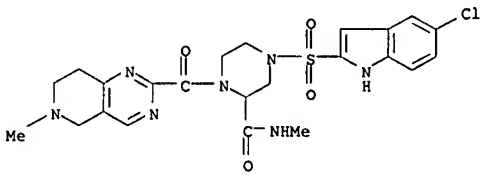


● HCl

RN 259806-48-9 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-N-methyl-1-[(4,5,6,7-tetrahydro-5-methyloxazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

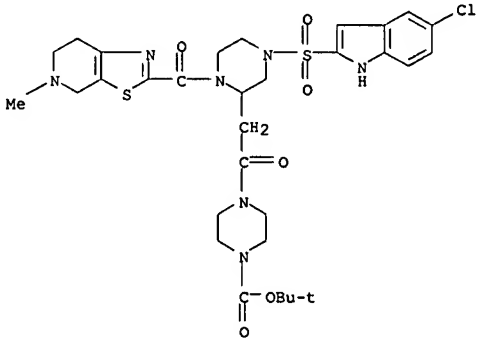


RN 259806-67-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[(5,6,7,8-tetrahydro-6-methylpyrido[4,3-d]pyrimidin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

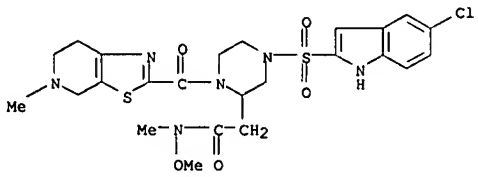


● HCl

RN 259806-89-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-2-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

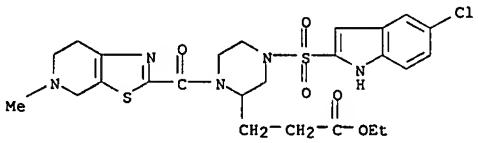


RN 259806-92-3 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methoxy-N-methyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

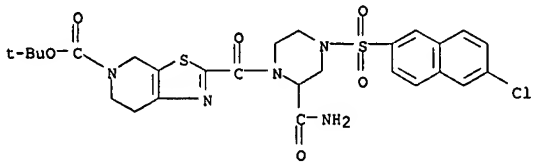


● HCl

RN 259807-04-0 CAPLUS
CN 2-Piperazinepropanoic acid, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



IT **222987-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonyl moiety-containing heterocyclic compds. as factor Xa inhibitors)
RN 222987-45-3 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:487215 CAPLUS
DOCUMENT NUMBER: 131:130007
TITLE: Substituted piperazinone derivatives and other oxoazaheterocyclyl compounds useful as factor Xa inhibitors
INVENTOR(S): Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls, Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aiwen; Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 300 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9937304	A1	19990729	WO 1999-US1682	19990127
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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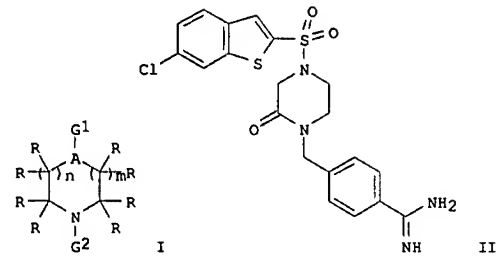
CA 2319198	AA	19990729	CA 1999-2319198	19990127
AU 9926533	A1	19990809	AU 1999-26533	19990127
AU 745425	B2	20020321		
BR 9907300	A	20001024	BR 1999-7300	19990127
EP 1051176	A1	20001115	EP 1999-906684	19990127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200002182	T2	20001221	TR 2000-200002182	19990127
JP 2002501024	T2	20020115	JP 2000-528286	19990127
EE 200000435	A	20020215	EE 2000-435	19990127
WO 2000032590	A1	20000608	WO 1999-US28074	19991124
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2003529531	T2	20031007	JP 2000-585232	19991124
NO 2000003808	A	20000926	NO 2000-3808	20000725
BG 104633	A	20010330	BG 2000-104633	20000725
US 2004102450	A1	20040527	US 2003-628093	20030725
PRIORITY APPLN. INFO.:			US 1998-72707P	A2 19980127
			US 1998-110012P	A2 19981125
			WO 1999-US1682	W 19990127
			US 1999-313611	A2 19990518
			US 1999-363196	A2 19990728
			WO 1999-US28074	W 19991124

OTHER SOURCE(S): MARPAT 131:130007
GI

102(e)

← 102(e)



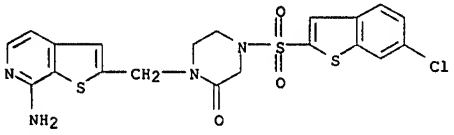
I

II

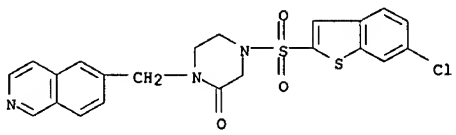
AB The invention is directed to oxoazaheterocyclyl compds. I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH, N; G1, G2 = (independently) -L-Cy; L = various atomic and mol. linkers, including O, (un)substituted NH or S, alk(en/yn)ylene, etc., or their combinations; Cy = (un)substituted (hetero)aryl, cycloalk(en)yl, heterocyclyl, etc.; R = (independently) H, CO2H, alkoxycarbonyl, (un)substituted carbamoyl, alkyl, (hetero)aryl, (hetero)aralkyl; or two geminal R groups = O or S; m, n = 0-2; with provisos]. The compds. inhibit factor Xa (no data), and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 780 compds. I, which are also claimed, and several hundred intermediates. For instance, sulfonamidation of 6-chlorobenzo[b]thiophene-2-sulfonyl chloride with 4-(2-oxopiperazin-1-ylmethyl)benzamidine bistrifluoroacetate (prepns. given) in CH2Cl2 in the presence of Et3N gave title compound II.

IT **234099-55-9P 234099-62-8P 234100-32-4P 234100-58-4P 234105-43-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa inhibitors)

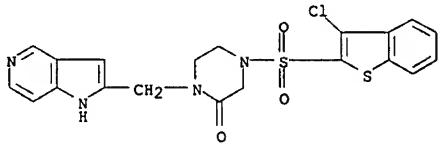
RN 234099-55-9 CAPLUS
CN Piperazinone, 1-[(7-aminothieno[2,3-c]pyridin-2-yl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]- (9CI) (CA INDEX NAME)



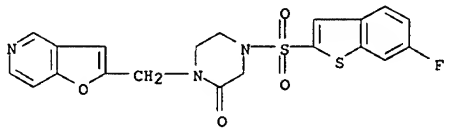
RN 234099-62-8 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(6-isoquinolinylmethyl)- (9CI) (CA INDEX NAME)



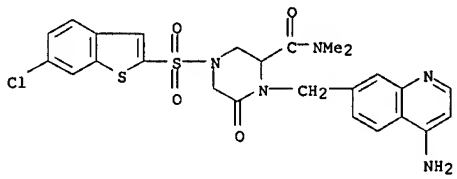
RN 234100-32-4 CAPLUS
CN Piperazinone, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234100-58-4 CAPLUS
CN Piperazinone, 4-[(6-fluorobenzo[b]thien-2-yl)sulfonyl]-1-(furo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234105-43-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-[(4-amino-7-quinolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:233901 CAPLUS
DOCUMENT NUMBER: 130:296694
TITLE: Preparation of heterocyclic compounds having the sulfonyl group as antithrombotics

INVENTOR(S): Kobayashi, Shozo; Komoriya, Satoshi; Ito, Masayuki; Nagata, Tsutomu; Mochizuki, Akiyoshi; Haginoya, Noriyasu; Nagahara, Takayasu; Horino, Haruhiko

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 342 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

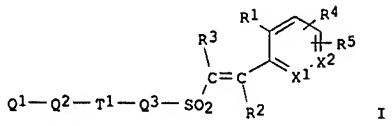
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9916747	A1	19990408	WO 1998-JP4411	19980930
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2304285	AA	19990408	CA 1998-2304285	19980930
AU 9892806	A1	19990423	AU 1998-92806	19980930
EP 1031563	A1	20000830	EP 1998-945542	19980930
EP 1031563	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
BR 9815377	A	20010116	BR 1998-15377	19980930
AT 314347	E	20060115	AT 1998-945542	19980930
US 6525042	B1	20030225	US 2000-508680	20000328
NO 2000001636	A	20000329	NO 2000-1636	20000329
US 2003232808	A1	20031218	US 2002-323978	20021220

PRIORITY APPLN. INFO.:

JP 1997-267117	A	19970930
WO 1998-JP4411	W	19980930
US 2000-508680	A3	20000328

OTHER SOURCE(S): MARPAT 130:296694

GI



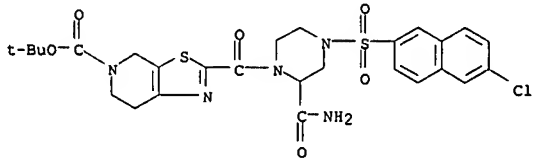
I

AB The title compds. I [R1 is hydrogen, hydroxyl, nitro or the like; R2 and R3 are each independently hydrogen, halogeno or the like; R4 and R5 are each independently hydrogen, halogeno or the like; Q1 is an optionally substituted saturated or unsatd. 5- or 6-membered cyclic hydrocarbon group or the like; Q2 is a single bond, oxygen or the like; Q3 is a heterocyclic moiety (represented by 4 generic structures); T1 is carbonyl or the like; and X1 and X2 are each independently methine or nitrogen] are prepared I speedily exert satisfactory and persistent antithrombotic effects through oral administration and cause few adverse effects. In an in vitro test for inhibition of activated blood coagulation factor X, 1-[(6-chloronaphthalen-2-yl)sulfonyl]-4-[(6-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]piperazine hydrochloride showed the Ki value of 6.6 nM.

IT **222987-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic compds. having the sulfonyl group as antithrombotics)

RN 222987-45-3 CAPLUS

CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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